

Pulse Detonation Rocket Engine Research at NASA Marshall

C. I. Morris

George C. Marshall Space Flight Center

Propulsion Research Center/TD40

Marshall Space Flight Center, AL 35812

Pulse detonation rocket engines (PDREs) offer potential performance improvements over conventional designs, but represent a challenging modeling task. A quasi 1-D, finite-rate chemistry CFD model for a PDRE is described and implemented. A parametric study of the effect of blowdown pressure ratio on the performance of an optimized, fixed PDRE nozzle configuration is reported. The results are compared to a steady-state rocket system using similar modeling assumptions.

Introduction

Pulse detonation rocket engines (PDREs) have generated considerable research interest in recent years¹ as a chemical propulsion system potentially offering improved performance and reduced complexity compared to conventional rocket engines. The detonative mode of combustion employed by these devices offers a thermodynamic advantage over the constant-pressure deflagrative combustion mode used in conventional rocket engines and gas turbines. However, while this theoretical advantage has spurred a great deal of interest in building PDRE devices, the unsteady blowdown process intrinsic to the PDRE has made realistic estimates of the actual propulsive performance problematic. The recent review article by Kailasanath² highlights some of the difficulties in comparing the available experimental measurements with numerical models.

In a previous paper by the author³, parametric studies of the performance of a single, straight-tube PDRE were reported. A 1-D, unsteady method of characteristics code, employing a constant- γ assumption behind the detonation front, was developed for that study. Models of this type are computationally inexpensive, and are particularly useful for parametric performance comparisons. For example, a plot showing the specific impulse of various PDRE and steady-state rocket engine (SSRE) configurations as a function of blowdown pressure ratio ($P_{\text{initial}}/P_{\text{final}}$) is shown in Figure 1. Note that the SSRE performance calculations employ the same constant- γ assumption used in the PDRE calculations. The performance curves indicate that a straight-tube PDRE provides superior specific impulse, compared to a SSRE with a sonic nozzle, over the entire range of pressure ratios. Note, however, that a straight-tube PDRE in general does not compare favorably to a SSRE fitted with an optimized converging-diverging (C-D) supersonic nozzle, particularly at the high pressure ratios typical for boost or in-space rocket applications.

This result is largely due to the choked outflow from a straight-tube PDRE. However, calculations of an ideal expansion of the PDRE outflow show that if a dynamically optimized supersonic nozzle could be fitted to a PDRE, then the specific impulse of the device would exceed that of a comparable SSRE. While such a nozzle is a considerable idealization, it is clear that nozzle design and optimization will play a critical role in whether the performance potential of PDREs can be effectively realized in practice.

The purpose of this paper is to report efforts at NASA Marshall Space Flight Center to study the effect of nozzles on PDRE gasdynamics and performance. Details of the quasi 1-D, finite-rate chemistry CFD model developed by the author are provided first. A parametric study of the effect of blowdown pressure

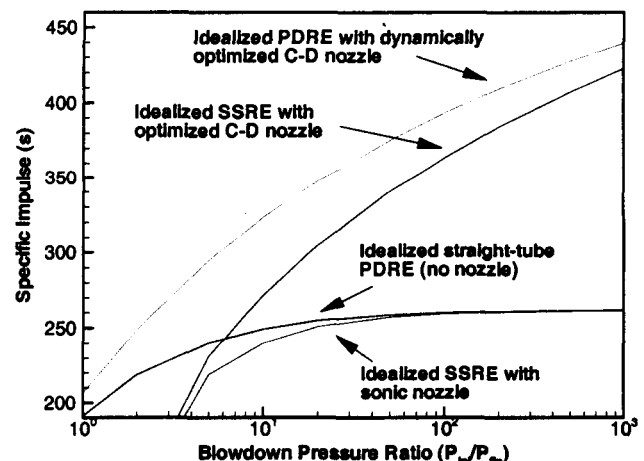


Figure 1: Performance comparison of a pulse detonation rocket engine (PDRE) with a conventional steady-state rocket engine (SSRE) equipped with both sonic and optimized supersonic converging-diverging nozzles. The specific heat ratio, γ , is held constant in all models. The final blowdown pressure in the PDRE is equal to the ambient pressure ($P_{\text{fin}} = P_{\text{amb}}$). Propellant mixture: stoichiometric $\text{H}_2\text{-O}_2$. Propellant initial conditions: $P_{\text{ini}} = 1$ atm, $T_{\text{ini}} = 300$ K.

ratio on the performance of an optimized, fixed PDRE nozzle configuration is then reported. The results are then compared to a SSRE system using similar modeling assumptions.

Theoretical Model

The PDRE system studied here is highly idealized, consisting of a constant-area (2.0 cm diameter) detonation tube 16 cm in length. One end is closed and the other end open to the environment, or attached to a simple conical converging-diverging nozzle section. The nozzle initially converges at a constant 14° angle to a throat 1.8 cm in diameter, and then diverges again at a constant 14° to a final exit diameter specified by the user. The computational domain automatically scales to fit the nozzle geometry. The detonation tube is pre-filled with a gaseous propellant mixture with no initial velocity. Stoichiometric $\text{H}_2\text{-O}_2$ at an initial pressure of 1 atm, and initial temperature of 300 K is utilized for all calculations in this work. An idealized, massless diaphragm isolates the propellant mixture from the nozzle and ambient environment until ruptured by the detonation wave. The nozzle section is initially filled with H_2 gas at the specified ambient pressure.

The time-dependent, finite-volume form of the quasi 1-D Euler equations is solved throughout the entire domain. A uniform grid spacing of $\Delta x = 0.1$ mm is utilized for all simulations in this study. The code utilizes a 1st-order time-step splitting approach in which the fluid and finite-rate chemistry solvers are called as separate subroutines. In the 1st-order approach, each complete time-step involves calling each subroutine once. As described by Oran and Boris⁴, the time-step splitting approach works well when relatively small time-steps are used.

The fluid solver used here is the explicit, 2nd-order accurate (in time and space), symmetric-TVD algorithm described by Yee⁵. The solver employs Roe's approximate Riemann solver modified for nonequilibrium ideal gases⁶. It also incorporates suggestions by Larrouturou⁷ to ensure species positivity. The ideal gas thermodynamic fits of McBride et al.⁸ are used for the 9 species in the problem (N_2 , O_2 , H_2 , OH , H_2O , H , O , HO_2 , and H_2O_2 are included).

The chemical solver utilizes the reduced 18-reaction $\text{H}_2\text{-O}_2$ ignition mechanism published by Petersen and Hanson⁹. As with most chemical kinetics problems, the time-integration of this mechanism

requires a stiff-ODE solver to ensure accuracy. The method used here is Newton iteration of a linearized implicit trapezoidal scheme. Typically, convergence to acceptable accuracy is achieved within 1-2 iterations at each time-step.

The detonation in each simulation is initiated by specifying elevated initial pressure and temperature conditions in the 20 cells adjacent to the closed wall. Pressures and temperatures 10 times larger the nominal fill values are used.

Ghost cells are utilized to specify the boundary conditions in the problem. A reflection-type boundary condition is utilized at the closed end of the detonation tube to simulate a solid wall. The method of characteristics¹⁰ is used to calculate the exit flow boundary condition. For sonic (choked) or supersonic exit flow, all exit flow properties are determined by the interior flow. For subsonic exit flow, the ambient pressure is specified and the method of characteristics is used to compute the remaining flow properties.

Two additional special restrictions are imposed in the simulations. In order to simulate the effect of an idealized diaphragm, only the detonation tube portion of the domain (from the closed wall to the diaphragm location) is computed initially. A reflection-type boundary condition is specified at the diaphragm location until the pressure in the adjacent cell rises 1.0% above the initial fill value. This special restriction is subsequently removed, and the entire domain is computed. Additionally, there is a check performed when the exit flow is supersonic. Since in this case the exit boundary conditions are entirely calculated from the interior flow, there is no way for the exit flow to return to a subsonic condition. Therefore, at each time step a check is made to determine if the pressure from standing normal shock at the exit is less than the ambient pressure. If true, then the normal shock properties are specified in the last interior cell, and a subsonic outflow boundary condition computed at the exit.

The time-dependent thrust is calculated at each time step by two different methods. One measure of the thrust assumes a control volume tightly bounding the solid surfaces of the PDRE, and is determined by integrating the pressure difference across all surfaces. A second measure assumes a rectangular control volume encapsulating the PDRE. This measure of thrust is determined from the sum of the time rate of change of the internal momentum integral across the domain, the

momentum flux from the nozzle section, and the pressure difference across the control volume. In general, there is excellent agreement between the two thrust calculations, and the time-integrated impulse determinations agree to within 0.1%. In all simulations, the calculation proceeds until the pressure at the closed end-wall is equal to the ambient pressure. Thus, these simulations should be thought of as single-shot results.

Results and Discussion

The blowdown pressure ratio is one of the most critical factors governing the performance of any rocket-type system. In this study, this parameter is defined as the ratio of the initial fill pressure in the detonation tube to the ambient pressure. The quasi 1-D CFD model is used to determine the optimum expansion ratio, ϵ , for a converging-diverging nozzle for a range of blowdown pressure ratios ranging from 1 – 100. At each pressure ratio, a variety of expansion ratios were tested, and a manual search was performed to determine the optimum expansion ratio. In each case, the optimum expansion ratio corresponds to the maximum total impulse. Two example cases will be examined in detail, followed by a comparison of the results among several systems over the entire pressure range.

The optimum nozzle exit diameter for the model PDRE system at a blowdown pressure ratio of 1.0 is found to be 2.2 cm. This corresponds to an expansion ratio of 1.49. Since the manual search for optimal exit radius was conducted in 1 mm increments, there is a variance on this expansion ratio of ± 0.26 . The mixture-based specific impulse of the optimized C-D system is 198.2 s. This is a modest improvement over the 192.9 s provided by the baseline detonation tube without any nozzle at this pressure ratio. A comparison between the single-shot thrust history for the optimized converging-diverging nozzle and the baseline detonation tube is shown in the upper panel of Figure 2. The corresponding exit pressure history is shown in the lower panel of the figure. It is evident from the thrust history that the reduced diameter of the throat in the C-D system increases the overall blowdown time compared to the baseline detonation tube. Additionally, the thrust for the optimized C-D system is actually lower than that of the baseline detonation tube for a significant portion of the early blowdown history. The main benefit of the C-D nozzle is derived from later in the blowdown history when the supersonic exit flow from the nozzle provides

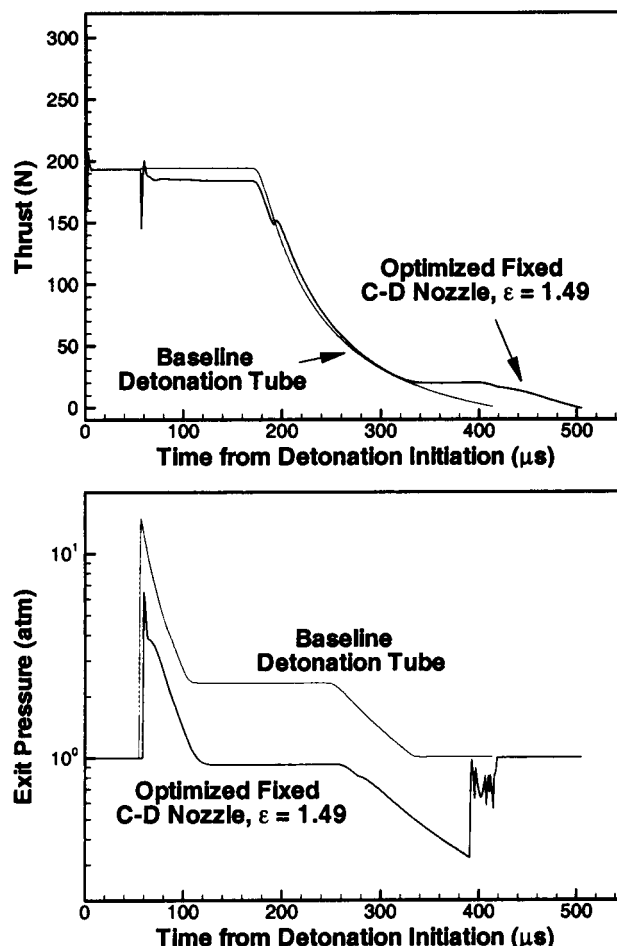


Figure 2: Comparison of thrust (upper panel) and exit pressure (lower panel) histories for PDRE systems at a blowdown pressure ratio of 1.0. Propellant mixture: stoichiometric $\text{H}_2\text{-O}_2$. Initial propellant conditions: $P_{\text{ini}} = 1 \text{ atm}$, $T_{\text{ini}} = 300 \text{ K}$.

slightly greater thrust than the choked flow of the baseline tube. Note that flow from the C-D nozzle becomes overexpanded late in the blowdown history, and eventually a normal shock forms at the exit by the procedure described in the previous section. It is evident that an optimized fixed C-D nozzle can provide only marginal benefit (2-3% additional specific impulse) over the baseline detonation tube at a blowdown pressure ratio of 1.0.

In contrast, substantial benefits can be realized from a C-D nozzle are larger blowdown pressure ratios. The optimum nozzle exit diameter for the model PDRE

system at a blowdown pressure ratio of 100.0 is found to be 8.2 ± 0.2 cm. This corresponds to an expansion ratio of 20.75 ± 1.0 . The mixture-based specific impulse of the optimized C-D system is 364.7 s, a significant improvement over the 261.0 s provided by the baseline detonation tube at this pressure ratio. A comparison between the single-shot thrust history for the optimized converging-diverging nozzle and the baseline detonation tube is shown in the upper panel of Figure 3. The corresponding exit pressure history is shown in the lower panel of the figure. As is evident from the figure, the blowdown process (to 0.01 atm) is considerably longer in this case than in the previous one. Note that the optimized C-D nozzle provides considerably higher thrust, compared to the baseline tube, throughout the blowdown history. This is due to familiar result from classical compressible flow that the best performance from a supersonic rocket nozzle is obtained when the pressure at the exit plane is expanded to the ambient value. As may be seen in the exit pressure history, the C-D nozzle expands the exhaust flow by roughly two orders of magnitude compared to the baseline tube. Thus, while the fixed nozzle cannot dynamically adapt to provide optimum expansion throughout the entire blowdown process, the resultant performance gain is still quite significant (~40%). It is worthwhile to note that the thrust provided by the C-D nozzle configuration is minimal for the last one-third of the blowdown history. This observation could provide useful guidance for performance optimization in a practical PDRE system.

The mixture-based specific impulse for both the baseline detonation tube, and the optimized fixed C-D nozzle system at each pressure ratio, is plotted for blowdown pressure ratios of 1.0, 2.0, 5.0, 10.0, 20.0, 50.0, and 100.0 in Figure 4. As would be expected from the example results discussed previously, the relative gain from the C-D nozzle system becomes more pronounced at higher pressure ratios.

It is instructive to compare the specific impulse of both PDRE systems with a SSRE under equivalent modeling assumptions. While frozen and equilibrium rocket performance calculations can be readily obtained from the NASA CET89 thermochemical code¹¹, these results are not directly comparable to the finite-rate chemistry model used in the current PDRE code. The primary concern is the tendency for chemistry to slow down in real nozzle systems as the temperature and pressure are reduced in the expansion process. Thus, it

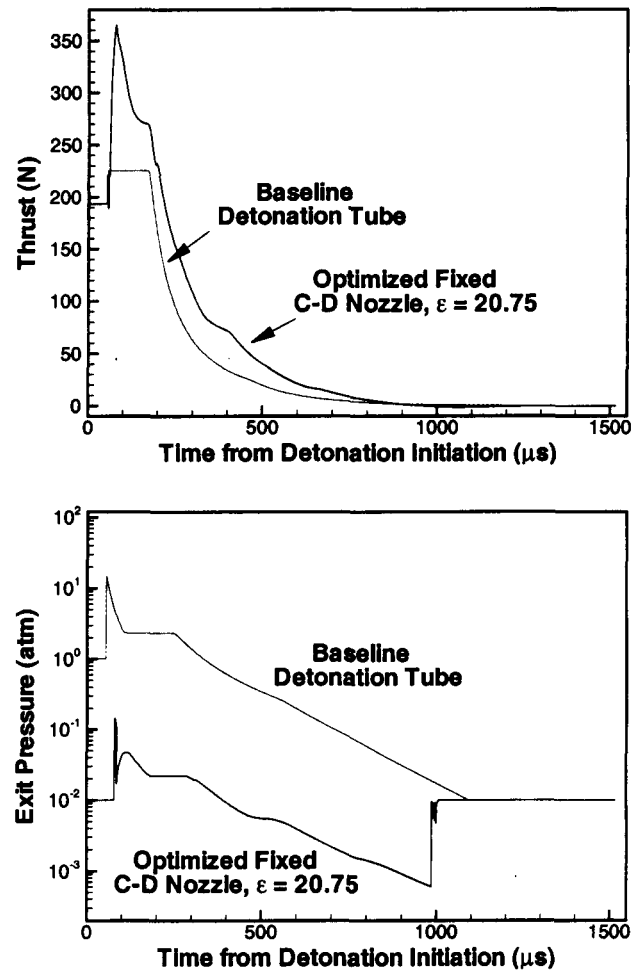


Figure 3: Comparison of thrust (upper panel) and exit pressure (lower panel) histories for PDRE systems at a blowdown pressure ratio of 100.0. Propellant mixture: stoichiometric $\text{H}_2\text{-O}_2$. Initial propellant conditions: $P_{\text{ini}} = 1$ atm, $T_{\text{ini}} = 300$ K.

is best to compare the finite-rate PDRE systems with a finite-rate SSRE model. This SSRE CFD model is heavily derived from the PDRE code. The 16 cm detonation tube is replaced with a thrust chamber 0.4 cm in length, and 3.6 cm in diameter. This thrust chamber then converges at a constant 14° angle to a throat 1.8 cm in diameter. After the throat, the nozzle again expands at 14° to the exit diameter specified by the user. The throat diameter and nozzle expansion rate are thus identical in both the PDRE and SSRE models. The equilibrium temperature, pressure and composition of stoichiometric $\text{H}_2\text{-O}_2$, burned at constant pressure and enthalpy (using CET89) from initial conditions of 300 K

and 1 atm, are fed as a constant enthalpy reservoir inflow boundary condition into the domain.

Similar to the PDRE nozzle optimization study, the finite-rate SSRE CFD model is run at various expansion ratios until the optimum specific impulse is obtained for a given pressure ratio. In each case, the SSRE model is run until the solution converges. In general, the specific impulse and optimum expansion ratio using finite-rate chemistry is slightly larger than that for frozen chemistry. Additionally, if the chemistry is frozen in the SSRE CFD model, there is excellent agreement (to within 0.5% in specific impulse) with the frozen-chemistry predictions of CET89.

When the finite-rate SSRE results are plotted in Fig. 4, we note that both the baseline and C-D nozzle PDRE systems outperform a SSRE at pressure ratios below ~ 7 . Thus, the PDRE may have considerable theoretical potential for rocket-type applications when the pressure of the ambient environment is high. Additionally, at higher blowdown pressure ratios, a PDRE with an optimized, fixed C-D nozzle has a greater specific impulse than an equivalent SSRE. This performance gain becomes relatively smaller at higher pressure ratios.

Summary and Future Work

A quasi 1-D, finite-rate chemistry CFD model for studying PDRE gasdynamics and performance is described and implemented. The performance of a simple fixed, but optimized, converging-diverging nozzle design is compared with a baseline detonation tube over a range of blowdown pressure ratios from 1 – 100. The results demonstrate that even relatively simple fixed nozzle designs can make significant improvements in PDRE performance at high pressure ratios.

Additional work is underway to study a wider range of nozzle configurations and pressure ratios, and to implement an ethylene chemistry model for comparison with experimental results from the literature.

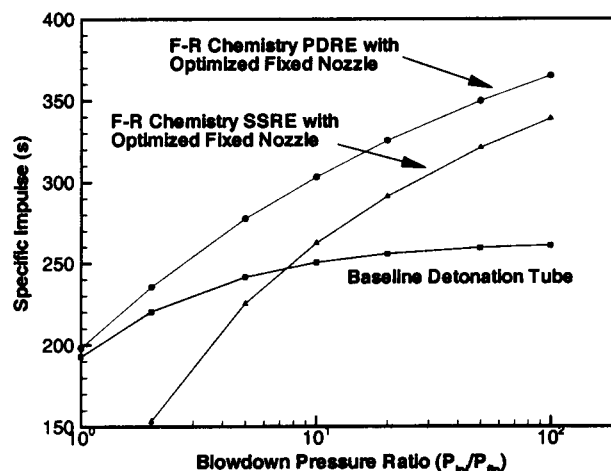


Figure 4: Performance comparison of various pulse detonation and steady-state rocket devices. All results obtained using finite-rate quasi 1-D CFD calculations. The final blowdown pressure in the PDRE is equal to the ambient pressure ($P_{fin} = P_{amb}$). Propellant mixture: stoichiometric H_2-O_2 . Propellant initial conditions: $P_{ini} = 1$ atm, $T_{ini} = 300$ K.

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Christopher Morris

Chris received his Ph.D. in Mechanical Engineering from Stanford University in 2001. Since then he has worked as a research engineer at the Propulsion Research Center at NASA Marshall Space Flight Center. Current research efforts involve studying pulse detonation rocket engines, and developing a high pressure combustor for studies of the rocket engine environment.

